# Engineering Design File

# Fate and Transport Modeling Results and Summary Report (60% Design Component)

# INEEL

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5.   Summary:

Fate and transport modeling was conducted to evaluate potential long-term concentrations in the Snake River Plain Aquifer that could result from contaminant transport from the INEEL CERCLA Disposal Facility.  Fate and transport simulations were conducted to identify contaminants of concern with respect to meeting groundwater remedial action objectives. Numerical modeling was performed using the STOMP computer code to identify dilution/attenuation factors for a suite of contaminants. These factors were subsequently applied to the remaining contaminants in the facility design basis inventory to identify those contaminants that may pose a potential risk and to prepare remedial action objective-based waste soil concentration limits. This report provides results from the contaminant screening evaluation and findings from fate and transport simulations.

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# ABSTRACT

This report describes the fate and transport modeling conducted to establish remedial action objective-based waste soil concentrations for design basis contaminants intended for disposal at the INEEL CERCLA Disposal Facility. The modeling results provide contaminant travel time and concentration at the point of compliance. The results are intended to provide guidelines for determining preliminary waste acceptance criteria for the ICDF list of potential contaminants of concern, and to evaluate design performance requirements of the ICDF cover barrier.

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# ACRONYMS

| | |
|---|---|
| CERCLA | Comprehensive Environmental Response, Compensation, and Liability Act |
| COC | contaminant of concern |
| EDF | Engineering Design File |
| EPA | Environmental Protection Agency |
| HEAST | Health Effects Assessment Summary Tables |
| ICDF | INEEL CERCLA Disposal Facility |
| INEEL | Idaho National Engineering and Environmental Laboratory |
| IRIS | Integrated Risk Information System |
| kg | kilogram |
| m | meter |
| m/yr | meters per year |
| MCL | maximum concentration level |
| MULTIMED | Multimedia Exposure Assessment Model |
| NCEA | National Center for Envrionmental Assessment |
| NCRP | National Council on Radiation Protection and Measurement |
| RBC | risk-based concentrations |
| RBL | risk-based level |
| RI/FS | Remedial Investigation/Feasibility Study |
| ROA | remedial action objectives |
| SRPA | Snake River Plain Aquifer |
| STOMP | Subsurface Transport Over Multiple Phases (transport modeling code) |
| WAG | waste area group |

# Fate and Transport Modeling Results and Summary Report

## 1. INTRODUCTION

The purpose of the contaminant transport simulations was to develop attenuation factors and travel time estimates for the contaminants of concern (COC) consistent with the facility design basis inventory presented in "INEEL CERCLA Disposal Facility Design Inventory," (DOE-ID 2001a). Performance of fate and transport modeling is primarily driven by the requirements of the Record of Decision (ROD). The scope of the modeling effort was limited to the constituents presented in the design inventory. The objectives of the modeling effort were as follows:

- To develop dilution/attenuation factors for use in evaluating travel times and resultant contaminant concentrations in groundwater at a compliance point downgradient of the ICDF facility.

- To develop a set of waste soil concentration limits based on meeting the groundwater remedial action objectives (ROA) of not exceeding maximum contaminant levels (MCLs) or risk-based concentrations (RBCs) in groundwater downgradient of the INEEL CERCLA Disposal Facility (ICDF).

- To evaluate the effectiveness of the planned final cover for the ICDF by utilizing the anticipated cover infiltration rate as one of the inputs for the contaminant fate and transport model.

- To support development of waste acceptance criteria by providing the RAO-based soil concentrations.

Several hydrologic investigations and modeling studies have been conducted. The current modeling effort incorporates the previous information as well as results of site-specific data collection activities and facility-specific design parameters to provide a conservative estimate of the transport scenarios in the vadose zone. Insufficient data exist to calibrate the model, especially considering the complexity of the vadose zone geology and other hydrologic features (e.g., the Big Lost River), and the time duration (1,000,000 years) is so great that the results contain a large degree of uncertainty. However, the information appears adequate for the purposes of setting waste soil concentration limits and acceptance criteria, and evaluating the effectiveness of the planned final cover.

Attenuation factors represent the ratio between the initial concentration of the contaminant in the waste and the resulting concentration in the aquifer at the compliance point. Travel time refers to the time elapsed from the placement of the waste in the ICDF to the arrival of the peak concentration of the contaminant at the compliance point. Travel time depends on the hydrologic properties of the porous media (e.g., infiltration rate, soil bulk density, and moisture content), the radiologic and environmental decay characteristics of the contaminants, and the adsorption characteristics of the contaminants as described by their distribution coefficient. Fate and transport of eight surrogate contaminants representing the expected range of contaminant distribution coefficients (and thus contaminant travel times) were simulated. The surrogates selected for the Tier 1 modeling and their respective distribution coefficients are shown in Table 1-1. Attenuation factors and travel time estimates for contaminants not specifically modeled may be estimated from the results of the contaminants with similar transport characteristics.

**Table 1-1.** Contaminant distribution coefficients and weighted averages for the different surrogates and model layer types.

| Model Layer Type | Distribution Coefficient ($K_d$) ($cm^3/g$) | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| | Surrogate 1 | Surrogate 2 | Surrogate 3 | Surrogate 4 | Surrogate 5 | Surrogate 6 | Surrogate 7 | Surrogate 8 |
| **Aquifer Layer** | | | | | | | | |
| SRPA basalt | 0 | 0 | 0.008 | 0.24 | 0.32 | 0.48 | 0.64 | 314 |
| **Vadose Zone Layer** | | | | | | | | |
| Basalt | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Interbed | 0 | 0 | 0.2 | 6 | 8 | 24 | 16 | 340 |
| Alluvium | 0 | 0 | 0.2 | 6 | 8 | 24 | 16 | 340 |
| Clay | 0 | 1 | 1 | 63 | 55 | 200 | 2400 | 340 |
| Operations layer | 0 | 0 | 0.2 | 6 | 8 | 24 | 16 | 340 |
| Waste | 0 | 0 | 0.2 | 6 | 8 | 12 | 16 | 340 |
| Weighted average* | 0.00 | 0.01 | 0.06 | 1.95 | 2.42 | 6.64 | 19.13 | 90.48 |

*The weighted average vadose zone $K_d$ is used only as an indicator of the relative mobility of specific contaminants in the vadose zone beneath the ICDF. The purpose of the weighted average $K_d$ is to group constituents with similar distribution coefficients in the vadose zone with the appropriate surrogate. The weighted average $K_d$ was computed by multiplying the fractional vadose zone thickness of each stratigraphic unit by the contaminant-specific $K_d$ for each unit and summing the results.

The point of compliance was located in the upper portion (approximately 5 m) of the Snake River Plain Aquifer (SRPA) 20 meters (m) downgradient from the ICDF landfill waste. Five recharge/infiltration rates were simulated to provide the range of expected results on the basis of barrier performance.

Existing hydrogeologic data and design specifications were used to provide input parameters for the fate and transport model. Sources of the data include previous modeling efforts (Martian 2000; Schafer et al. 1997), the Waste Area Group 3 Geotechnical Report (DOE-ID 2000), and input from the design requirements. Transport characteristics (distribution coefficients [$K_d$]) for the COC were previously inventoried for the vicinity of the ICDF (Jenkins 2001[a]). The distribution coefficients are included in the contaminant-specific information presented in Appendices A and B for radiological and non-radiological contaminants, respectively.

The fate and transport modeling effort is divided into two activities. The first (Tier 1) activity is presented in this report and is intended to screen the design inventory contaminants based on the apparent risk posed by the contaminants at the downgradient aquifer compliance point. The Tier 1 screening will identify contaminants that present the dominant portion of the apparent risk and support establishing preliminary upper bounds on acceptable concentrations of minor constituents in the design inventory.

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[a] Jenkins, T., DOE, letter to Martin Doornbos, BBWI, July 3, 2001, *$K_d$ values for INTEC groundwater modeling (EM-ER-01-115)*.

The Tier 1 fate and transport modeling utilized the physical conceptual model of the current ICDF design and introduced only the distribution coefficient and expected natural decay (e.g., radioactive decay for radioisotopes and environmental half-life for organic compounds) as attenuating factors. The Tier 1 simulations were conducted at steady-state recharge conditions at five selected rates to encompass the natural, ambient, recharge at the site, and the expected effective rate of the final facility cover.

The subsequent Tier 2 fate and transport modeling may be conducted to further evaluate the waste constituents that provide the majority of the apparent risk. The Tier 2 simulations will be presented in the 90% design documents and will incorporate the following additional factors:

- Potential limitations to initial solubility of constituents in the landfill leachate as controlled by the geochemistry of waste soil

- Effects of removal of constituent mass from the waste soil by active leachate pumping during the design post-closure period.

# 2.  FATE AND TRANSPORT MODELING METHODS

## 2.1   Modeling Approach

The following section describes the methods used to simulate the fate and transport of COC identified for disposal at the ICDF. The two-dimensional (vertical and horizontal parallel to groundwater flow) numerical model used to simulate the contaminant transport from the ICDF was developed according to the conceptual model presented in the report describing the screening model results (Martian 2000) and additional information regarding the construction of the ICDF itself.

The modeling effort used the STOMP version 2.0 (Subsurface Transport Over Multiple Phases) finite difference code developed by Pacific Northwest National Laboratory (PNNL) to conduct the simulations. A description of the STOMP code is found in the Theory Guide (PNNL 1996) and the User's Guide (PNNL 2000). An evaluation of vadose zone model codes recently conducted at the Hanford Site (Mann et al. 1999) ultimately resulted in the selection of STOMP for simulating high-level radioactive tank waste fate and transport (Mann 2001[b]). STOMP also may include aquifer fate and transport so that the vadose and aquifer portions of the modeling may be conducted within one model domain.

Quantitative predictions of hydrogeologic flow and contaminant transport are generated from the numerical solution of non-linear partial differential equations that describe subsurface environment flow and transport phenomena. STOMP capabilities include, among others, the simulation of saturated and unsaturated flow regimes, transport of radioactive elements and non-decaying contaminants, and transport of aqueous phase organic compounds. A complete description of STOMP capabilities and the actual equations and the partial differential approximations are contained within the Theory Guide and User's Guide, and the Applications Guide (Nichols et al. 2000) provides information regarding code validation.

The screening model and results (Martian 2000) provided a means of validating the STOMP model and modeling approach. A two-dimensional model using similar input as the screening model was constructed using STOMP. The STOMP model simulated the screening model described as possessing an attenuation barrier. To account for the side slopes of the ICDF, the recharge was proportioned according to the increase in ICDF area at ground surface. The screening model identified square bottom dimensions of 125 m, and square ground surface dimensions of 155 m. Thus, recharge through the ICDF in the STOMP model was proportioned by a factor of 1.5376 (155 m × 155 m/[125 m × 125 m]). Table 2-1 shows the comparison of the STOMP and the screening model results. The STOMP results compared well to the screening model results; in general, peak concentrations and arrival times were within 10%.

One difficulty encountered in matching the screening model output was imitating in STOMP the hydraulic characteristics of the basalt layers in the screening model (TETRAD). The Brooks-Corey equation algorithm used in TETRAD to describe the basalt layers' moisture content (saturation)-capillary pressure relationship (and the assumed linear relationship between saturation and relative hydraulic conductivity) appears to be proprietary, and is not directly available in STOMP. However, the algorithm can be approximated in STOMP by calculating and tabulating saturation-capillary pressure values and interpolating between tabulated values. The results presented in Table 2-1 show that changing the saturation-capillary pressure relationship from the version of the Brooks-Corey equation in TETRAD to the van Genuchten equation resulted in little change in the peak concentration or peak arrival time.

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[b] Frederick Mann, CH2M HILL, to McMahon, William J., CH2M HILL, November 5, 2001, "Information regarding RFP," (Stomp Requirements).

Because the van Genuchten saturation-capillary pressure relationship is more widely available for vadose modeling than the version of the Brooks-Corey equation used in TETRAD (e. g., neither HYDRUS or STOMP include it, nor is that version of the Brooks-Corey equation contained in EPA/600/2-91/065 [1991]), the fate and transport simulations used the van Genuchten equation to simulate the basalt moisture content (saturation)-capillary pressure relationship. The SRPA basalt and vadose basalt van Genuchten curve fit parameters were determined by approximating the saturation-capillary relationship shown in Figure 2-21 of Schafer et al. (1997) with van Genuchten saturation-capillary pressure curves (see Figure 2-1).
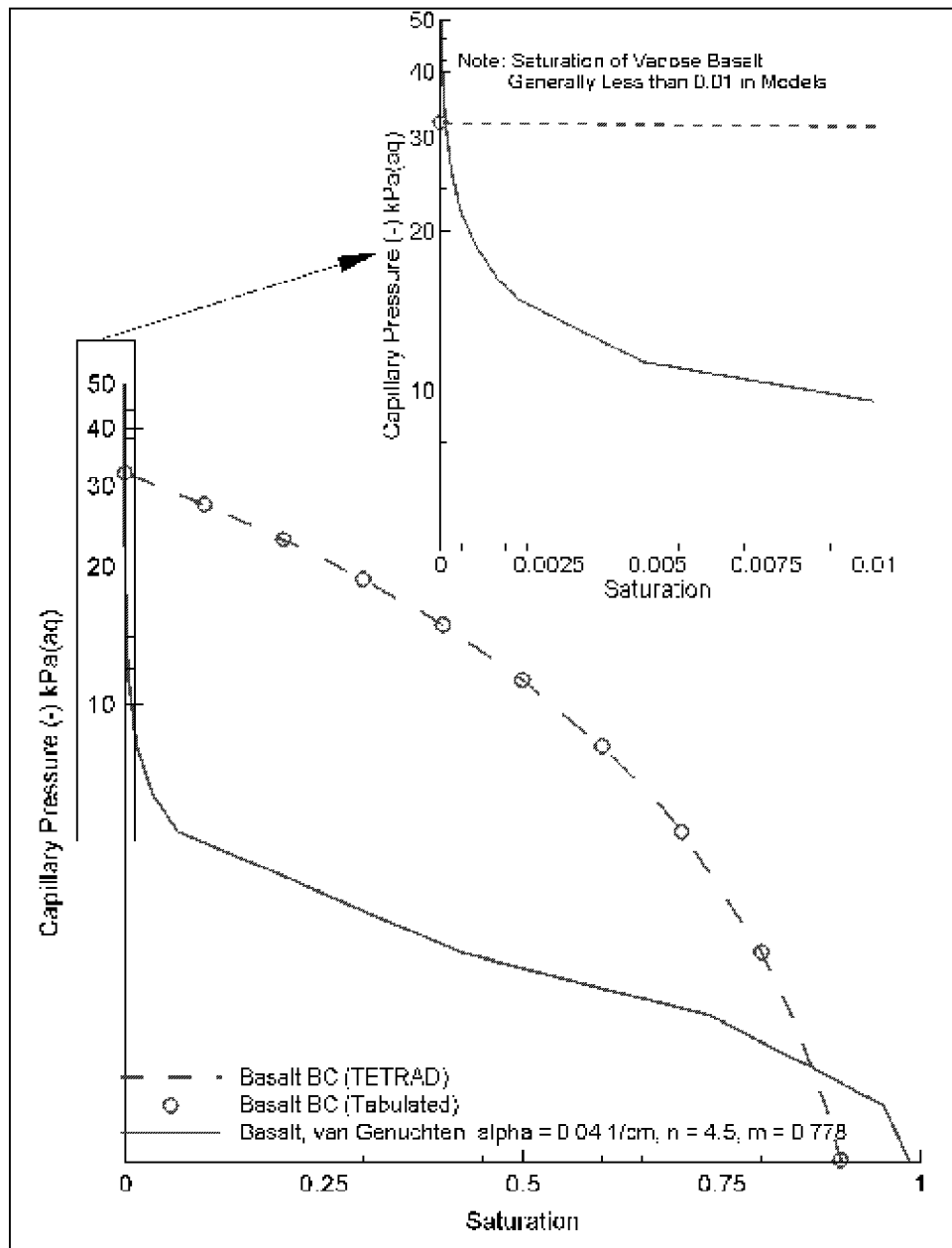


**Figure 2-1.** Comparison of the van Genuchten moisture content (saturation)-capillary pressure relationship to the TETRAD Brooks-Corey equation.

Usually the m parameter determined from the saturation-capillary pressure relationship is also used in the Mualem relative hydraulic conductivity equation, but using a value of 1.9 (instead of 0.778) provided a closer approximation of the assumed linear relationship between saturation and relative hydraulic conductivity.

Figure 2-2 shows the revised conceptual model used to develop the numerical model grid (shown in Figure 2-3) and establish the model layers. Similar to the screening model, the numerical model only accounts for the vertical transport of moisture and contaminants in the vadose zone, and assumes that there is no influence from the wastewater disposal ponds or the Big Lost River. The length dimension of the ICDF facility in the numerical model was determined from preliminary construction drawings (DOE 2001b) to be about 160 m in the direction parallel to groundwater flow. In the direction perpendicular to flow, the length dimension is about 194 m. The side slope of the facility is ~3:1, so for the estimated waste volume (510,000 $yd^3$ or 389,923 $m^3$), the height of the trapezoidal waste volume is about 9.3 m. The slope of the sides increases the area at the top of the waste area to about 215.8 m by 249.8 m. Therefore, the contaminant transport portion of the modeling increased the specified recharge rate by a factor of ~ 1.74:1 (215.8 m × 249.8 m/[160 m × 194 m]). To maintain waste volume balance in the numerical model, the simulated waste height was adjusted to 12.56 m (389,923 $m^3$/ [160 m × 194 m] $\cong$ 12.56 m). The two-dimensional model domain represented a vertical cross-section of the ICDF waste area and operations area, the clay liner, the vadose zone, and 20 m to the compliance point within the upper portion (approximately 5 m) of the SRPA.

The hydraulic and contaminant fate and transport modeling was conducted in two steps. The first step involved inputting background hydraulic boundary conditions and calculating the steady-state solution for water content and capillary pressure. The upper boundary received constant infiltration equal to 0.01 m/yr (1 cm/yr), and the sides of the model in the vadose zone allowed no flow or contaminant transport to occur across those boundaries. The upgradient aquifer boundary received a constant flux of 0.06 m per day (m/day), which equates to a flow velocity of 1 m/day. The downgradient aquifer boundary was fixed to a constant hydraulic head such that the head at the compliance point equaled approximately 5 m. The background hydraulic boundary conditions were comparable to those presented in Martian (2000). The output solution of the steady-state simulation was used as the input starting conditions for the contaminant transport simulations. Figure 2-4 shows the residual moisture content of the STOMP simulation.

Contaminant attenuation factors for eight surrogates representing the range of expected distribution coefficients were calculated in the following manner. The waste layers of the model were assigned unit contaminant concentrations (1 unit of contaminant per kilogram of waste soil). The waste layer contaminant concentrations were assumed to occur instantaneously, but depleted over time as contaminant mass exited the waste layers. Using unit contaminant concentrations in the waste soil allows the resulting aquifer concentrations at the compliance point (units/L) to be scaled according to the actual waste concentrations based on the design inventory of the ICDF. For example, if 1 unit of contaminant per kilogram of waste soil resulted in a peak concentration of 0.005 units/L of contaminant at the compliance point, then an ICDF inventory of 3 mg contaminant per kilogram of waste soil would result in a concentration of 0.015 milligram per liter (mg/L) at the compliance point. Conversely, acceptable concentration limits in the ICDF waste may be back-calculated by dividing the allowable concentration in the aquifer by the resulting aquifer concentration from the model. Radioactive decay was not included in this step of the modeling.

To determine the dilution/attenuation factor and actual peak concentration at the compliance point (according to the model results), the scaled concentration at each time in the model simulation is multiplied by the radioactive or environmental decay rate. An example of this method is shown in Figure 2-5, which shows the concentration of Surrogate 4 and three of the uranium isotopes at the compliance

point at the design recharge/infiltration rate. Uranium-238, with a half life of 4.47E+09 years, experiences virtually no decay during the simulation period, and thus the peak concentration and arrival time are essentially equivalent to those of the undecayed surrogate. The shorter lived isotopes tend to peak earlier, but at much lower concentrations than the surrogate or longer lived isotopes. Contaminant transport was modeled at five recharge/infiltration rates (0.01, 0.001, 0.0005, 0.0001, and 0.00005 meters per year [m/yr]) to provide a sensitivity analysis on the range of expected results on the basis of barrier performance.



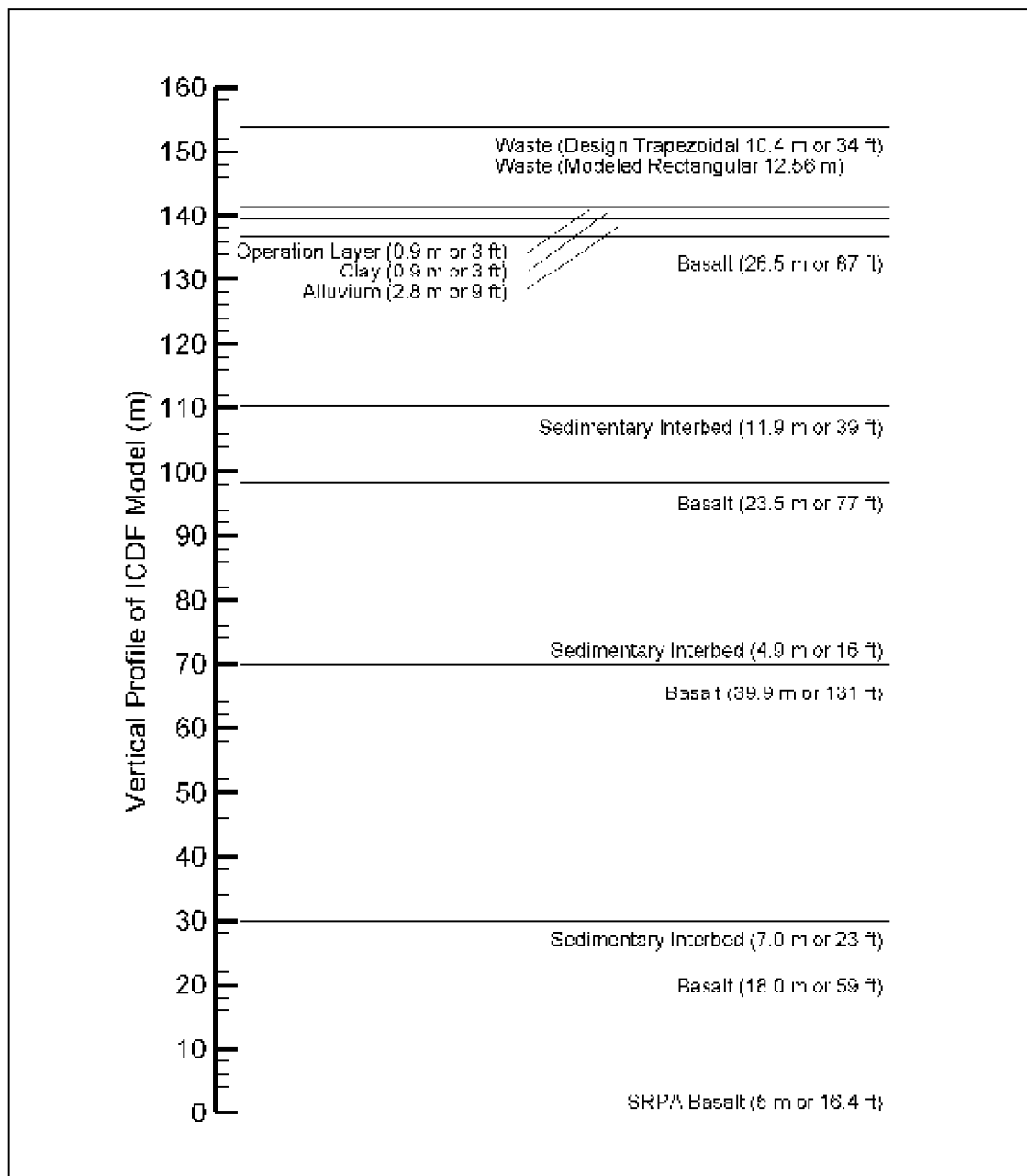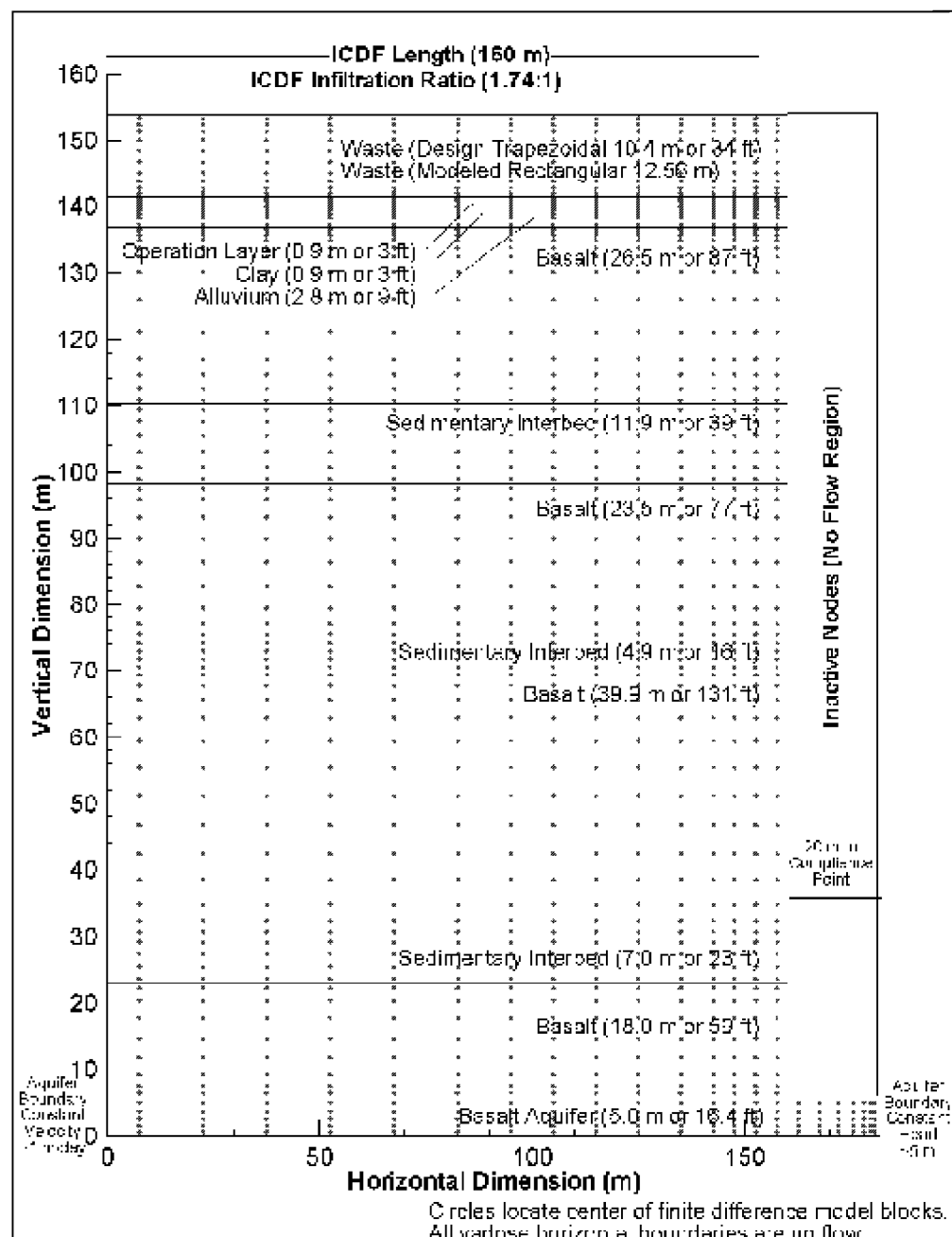**Figure 2-2.** Conceptual model of ICDF vertical profile.

**Figure 2-3.** Numerical model grid and boundary conditions of ICDF vertical profile.
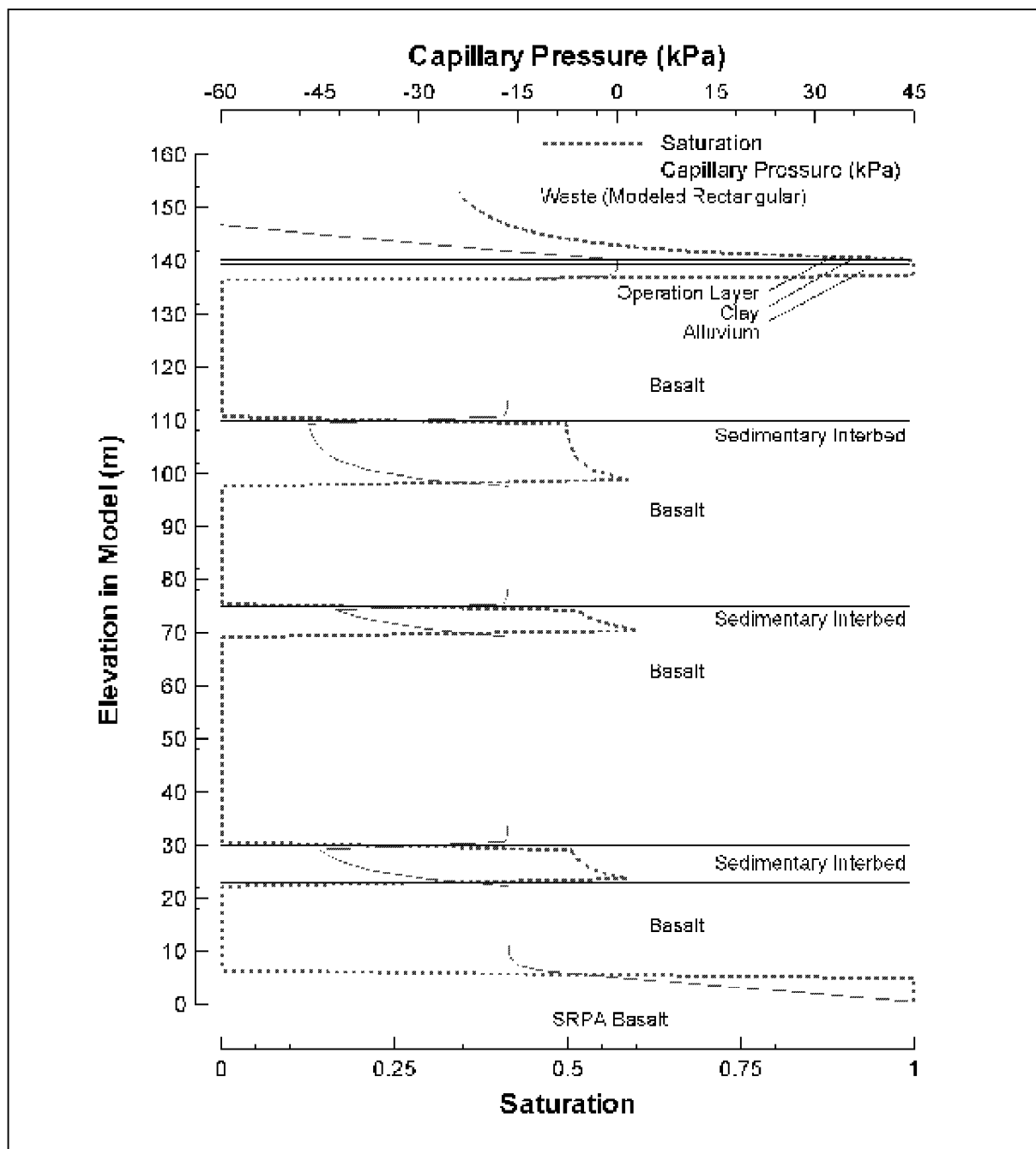
**Figure 2-4.** Residual moisture and capillary pressure initial conditions for transport simulations using STOMP.
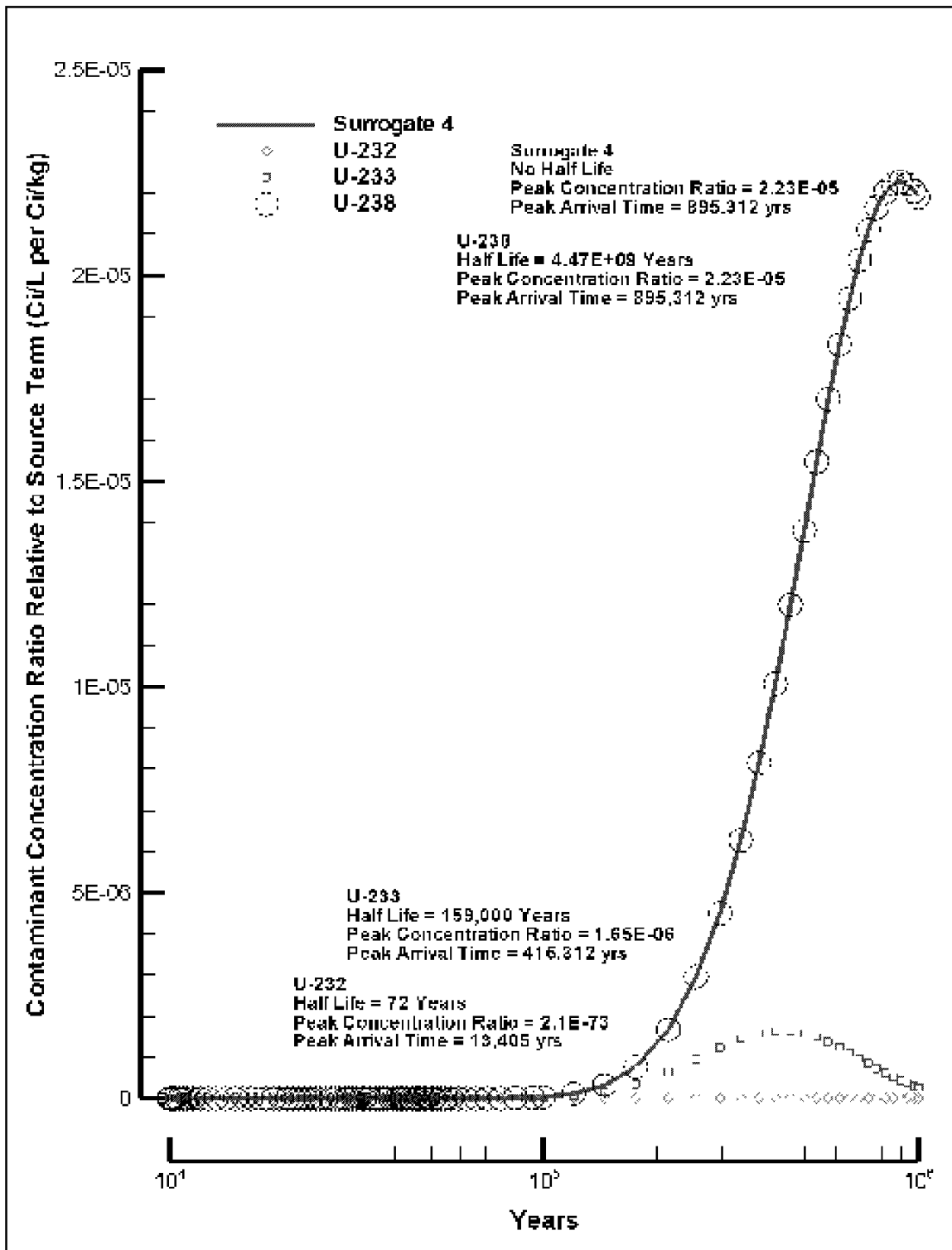
**Figure 2-5.** Example contaminant arrival curves at the compliance point for Surrogate 4 and three uranium isotopes at the design recharge/infiltration rate.

Simulating water and contaminant transport through the vadose zone requires the solution of the non-linear partial differential equations used to describe flow through unsaturated porous media. Solution of the equations requires moisture retention (aqueous phase pressure and moisture content) and fluid transport (hydraulic conductivity and moisture content or aqueous phase pressure) characteristic data for the porous media contained within the model domain. The model uses functional relationships (referred to as characteristic curves) to describe the characteristic data. The equation (1) used in the model (as presented in PNNL 1996) and shown below was developed by van Genuchten to describe the moisture retention characteristic of the porous media:

$$S_w = \{1 + (\alpha[\frac{P_g - P_w}{\rho_w g}])^n\}^{-m} \quad for\ P_g - P_w > 0$$

$$S_w = 1 \quad for\ P_g - P_w \leq 0$$

(1)

Where

$S_w$ = degree of water saturation of the porous media (dimensionless)

$P_g$ = absolute pressure of the gas phase present (Pa, atmospheric pressure for these simulations)

$P_w$ = absolute pressure of the water phase present (Pa)

$\rho_w$ = density of water (kg/m$^3$)

g = acceleration of gravity (m/s$^2$)

$\alpha$ (1/m), n, and m are curve fit parameters, and m = 1 - 1/n except for basalt.

The Mualem equation (as presented in PNNL 1996 and shown below) was used to describe hydraulic conductivity as a function of moisture content:

$$k_{rw} = (S_w)^{1/2} \{1 - (1 - [S_w]^{1/m})^m\}^2 \quad and$$

$$K = k_{rw} * K_{sat}$$

(2)

Where

K = permeability (cm$^2$) or hydraulic conductivity (cm/s)

$k_{rw}$ = relative permeability or hydraulic conductivity

$K_{sat}$ = permeability (cm$^2$) or saturated hydraulic conductivity (cm/s)

$S_w$ and m are defined as before.

The results of the comparison of the screening model (Martian 2000) to the STOMP simulation using the same input parameters is presented in Table 2-1. This comparison indicates good correlation of both travel times and groundwater contaminant concentrations between the two simulations for the contaminants identified.

**Table 2-1.** Comparison of STOMP and screening model results (EDF-ER-170 2000) with attenuation barrier at ICDF bounding inventory values.

| | STOMP Results | | | | Screening Model Results | |
|---|---|---|---|---|---|---|
| | Recharge Rate 1.0 cm/yr | | | | | |
| | Using Approximated TETRAD Brooks-Corey Basalt Saturation-Capillary Pressure Relationship | | Using van Genuchten Basalt Saturation-Capillary Pressure Relationship | | Using TETRAD Brooks-Corey Basalt Saturation-Capillary Pressure Relationship | |
| Contaminant | Peak Concentration (pCi/L) | Peak Arrival Time (Years) | Peak Concentration (pCi/L) | Peak Arrival Time (Years) | Peak Concentration (pCi/L) | Peak Arrival Time (Years) |
| I-129 | 65.4 | 561 | 63.8 | 581 | 64.8 | 600 |
| Np-237 | 57.4 | 14,348 | 56.1 | 15,348 | 59.5 | 15,450 |
| Tc-99 | 19,150 | 813 | 18,634 | 834 | 20,500 | 800 |
| | Recharge Rate 0.1 cm/yr | | | | | |
| I-129 | 7.05 | 4,080 | 6.93 | 5,010 | 7.08 | 5,400 |
| Np-237 | 5.92 | 125,802 | 5.82 | 125,802 | 4.99 | >100,000 |
| Tc-99 | 2,034 | 7,048 | 1,991 | 7,248 | 2,220 | 8,400 |

Table 2-2 presents the soil hydraulic and contaminant transport parameters of the different layers used in the model and the source of the information. In general, parameters developed in previous models (e.g., Schafer et al. 1997; EDF-ER-170 2000) were carried forward except where new data were available. The site geotechnical report (DOE-ID 2000) provided substantial new information and data from the lower alluvium unit present near the ICDF site, and the design specifications provided new information regarding the clay, operations layer, and waste layer. Table 2-3 presents the hydraulic properties for the different layers. The saturated moisture content of each model layer type was assumed to equal the porosity. Synthetic materials that are part of the liner design (e.g., polymer membranes, etc.) were not included in the model stratigraphy.

**Table 2-2.** Summary of soil properties and moisture content (saturation)-aqueous pressure relationship curve fit parameters.

| Model Layer Type | Saturated Moisture Content | Residual Moisture Content | Curve Fit Parameter α (1/m) | Curve Fit Parameter n | Curve Fit Parameter m |
|---|---|---|---|---|---|
| SRPA basalt[a] | 0.06 | 0.0002 | 4.0 | 4.50 | 0.778 / 1.9 |
| Basalt[l] | 0.05 | 0.0002 | 4.0 | 4.50 | 0.778 / 1.9 |
| Interbed[b] | 0.487 | 0.142 | 1.066 | 1.523 | 0.343 |
| Alluvium[c,] | 0.424 | 0.142 | 0.595 | 1.108 | 0.097 |
| | [0.487]* | | [1.066]* | [1.523]* | [0.343]* |
| Clay[d,] | 0.39 | 0.07 | 0.800 | 1.090 | 0.083 |
| | [0.4]* | | | | |

**Table 2-2.** (continued).

| Model Layer Type | Saturated Moisture Content | Residual Moisture Content | Curve Fit Parameter α (1/m) | Curve Fit Parameter n | Curve Fit Parameter m |
|---|---|---|---|---|---|
| Operations layer[e] | 0.275 | 0.083 | 1.066 | 1.523 | 0.343 |
| | [0.487]* | [0.142]* | | | |
| Waste[e] | 0.266 | 0.072 | 1.066 | 1.523 | 0.343 |
| | [0.487]* | [0.142]* | | | |

a.  Basalt curve fit parameters moisture content parameters are reported in Schafer et al., 1997, and curve fit parameters are estimated from moisture content/pressure relationship in Shafer et al., 1997. Basalt parameter m is 0.778 for saturation-capillary pressure relationship, and 1.9 for saturation-relative hydraulic conductivity relationship.

b.  Interbed moisture content and curve fit parameters are reported in Schafer et al., 1997.

c.  Alluvium parameters are determined from site geotechnical report (DOE-ID 2000), except the residual moisture content (no data reported).

d.  Clay saturated moisture content is based on design specifications; residual moisture content and curve fit parameters are reported in EDF-ER-170, 2000.

e.  Operations and waste layers saturated and residual moisture content parameters are based on design specifications; curve fit parameters are reported in EDF-ER-170, 2000.

*  Values used in the screening model (EDF-ER-170 2000) are shown in brackets where different.

**Table 2-3.** Summary of soil hydraulic and contaminant transport properties.

| Model Layer Type | Bulk Density[a] (kg/m³) | Saturated Hydraulic Vertical Conductivity[b] (cm/s) | Longitudinal Dispersivity[c] (m) | Transverse Dispersivity[c] (m) |
|---|---|---|---|---|
| SRPA basalt | 2491 | 2.6e-04[d] | 6 | 3 |
| Basalt | 2518 | 2.6e-04[d] | 5 | 0 |
| Interbed | 1359 | 6.7e-05 | 5 | 0 |
| Alluvium | 1526 | 6.7e-08 | 5 | 0 |
| Clay | 1586 | 1e-07 | 5 | 0 |
| Operations layer | 1922 | 1e-04 | 5 | 0 |
| Waste | 1946 | 1e-03 | 5 | 0 |

a.  Bulk density is determined from the saturated moisture content and assumed particle solid density of 2650 kg/m³, except for alluvium with bulk density values reported in the site geotechnical report (DOE-ID 2000), and the clay with a design particle solid density of 2600 kg/m³.

b.  Saturated hydraulic conductivity values are reported in EDF-ER-170 (2000), except for alluvium with values reported in DOE/ID (2000), and basalt with values reported in Schafer et al., 1997.

c.  Longitudinal and transverse dispersivity values are reported in EDF-ER-170 (2000).

d.  Basalt saturated horizontal hydraulic conductivity = 7.7e-02 cm/sec.

## 2.2 Model Results

The STOMP simulations were extended to a maximum elapsed time of 1 million years. The results show that no undecayed surrogate peaks reached the compliance point in less than 30,000 years at the maximum design infiltration rate of 0.0001 m/yr (based on the results of hydrologic modeling of the final cover design for the ICDF). Only surrogates with weighted vadose distribution coefficients less than or equal to that of Surrogate 4 will peak at the compliance point in less than 1 million years at the maximum design infiltration rate. Radionuclide contaminant concentrations may peak at the compliance point before the arrival of the undecayed surrogate peak. However, the dilution/attenuation factor for these radionuclides tends to be orders of magnitude less than the dilution/attenuation factor of the undecayed surrogate. The results indicate that almost any radionuclide with a half life less than 1,000 years will not reach the compliance point before decaying to undetectable quantities.

The dilution/attenuation factors shown in Table 2-4 indicate that the ratio of the concentration in groundwater at the compliance point to the concentration in the ICDF (the attenuation factor) of the most mobile constituent (Surrogate 1) is 8.04e-04. This means that for a non-decaying contaminant, the peak groundwater concentration (in mg/L or pCi/L) at the compliance point will be 1.2e+03 times (1/8.04e-04) less than the soil concentration in the ICDF in mg/kg or pCi/kg. The peak concentration of the most mobile non-decaying constituents is expected to occur at least 32,605 years after placement of the waste. Tritium is an example of a radionuclide simulated by Surrogate 1. Because the half life of tritium is 12.3 years, the peak concentration of that contaminant occurs closer to the contaminant's first arrival (70 years, as indicated in the STOMP results) than the arrival of the undecayed peak, but the dilution/attenuation factor is less by several orders of magnitude. Results of the sensitivity study evaluating peak concentration and arrival times at four other recharge rates are presented in Appendix A.

Table 2-4 presents the results of the contaminant transport modeling of peak arrival time and peak concentration for all five simulated recharge rates. Graphical depiction of the trends of the modeled contaminant concentrations in the downgradient groundwater compliance point are shown in Appendix A. These trend charts are normalized to full scale and the order-of-magnitude changes in the vertical (concentration) axis should be noted. By using the attenuation factor derived from the simulations to scale the design inventory concentrations, the estimated compliance point concentration of the modeled constituents can be calculated as shown in Table 2-5. The dilution/attenuation factors and subsequent estimates of decayed concentrations are presented in Appendix B for radionuclides and non-radioactive contaminants.

**Table 2-4.** Results of Tier 1 surrogate contaminant transport simulations and example radionuclide dilution/attenuation factors and peak arrival times at maximum design recharge rate.

| | Recharge Rate 0.0001 m/yr | |
|---|---|---|
| | Dilution/Attenuation Factor (Peak Concentration) | Peak Arrival Time |
| Contaminant | (1/L per 1/kg soil) | (yrs) |
| Surrogate 1 | 8.04E-04 | 32,605 |
| H-3 | 5.30E-12 | 70 |
| Surrogate 2 | 6.70E-04 | 36,605 |
| I-129 | 6.68E-04 | 36,605 |
| Surrogate 3 | 4.23E-04 | 59,007 |
| Tc-99 | 3.50E-04 | 56,566 |

Table 2-4. (continued)

| | Recharge Rate 0.0001 m/yr | |
| | Dilution/Attenuation Factor (Peak Concentration) | Peak Arrival Time |
| Contaminant | (1/L per 1/kg soil) | (yrs) |
| --- | --- | --- |
| Surrogate 4 | 2.23E-05 | 895,312 |
| U-235 | 2.23E-05 | 895,312 |
| Surrogate 5 | 1.76E-05 | 1,000,000 |
| Np-237 | 1.27E-05 | 1,000,000 |
| Surrogate 6 | 1.32E-06 | 1,000,000 |
| Sr-90 | 0.00E+00 | No Arrival |
| Surrogate 7 | 3.64E-07 | 1,000,000 |
| Pu-239 | 3.88E-12 | 180,000 |
| Surrogate 8 | 3.18E-15 | 1,000,000 |
| Am-241 | 0.00E+00 | 280,000 |

**Table 2-5.** Results of selected contaminant transport simulations at maximum design recharge rate scaled to ICDF inventory.

| | | | Compliance Point Peak Concentration – decayed (pCi/L) | |
| | | ICDF Inventory (Ci/kg or mg/kg) | Infiltration/Recharge Rate (0.0001 m/yr) | |
| Contaminant [Surrogate] | Half-Life (yrs) | | DAF (Ci/L per Ci/kg or mg/L per mg/kg) | pCi/L or mg/L |
| --- | --- | --- | --- | --- |
| H-3 [Surrogate 1] | 1.230E+01 | 4.96E-08 | 5.30E-12 | 2.63E-07 |
| I-129 [Surrogate 2] | 1.570E+07 | 1.30E-09 | 6.68E-04 | 8.68E-01 |
| Tc-99 [Surrogate 3] | 2.130E+05 | 5.76E-09 | 3.50E-04 | 2.02E+00 |
| U-235 [Surrogate 4] | 7.040E+08 | 1.10E-10 | 2.23E-05 | 2.45E-03 |
| Np-237 [Surrogate 5] | 2.140E+06 | 6.43E-10 | 1.27E-05 | 8.19E-03 |
| Sr-90 [Surrogate 6] | 2.910E+01 | 2.29E-05 | 0.00E+00 | 0.00E+00 |
| Pu-239 [Surrogate 7] | 2.410E+04 | 6.66E-09 | 3.88E-04 | 2.58E-08 |
| Am-241 [Surrogate 8] | 4.327E+02 | 1.76E-07 | 0.00E+00 | 0.00E+00 |
| As [Surrogate 3] | N/A | 5.65E+00 | 4.23E-04 | 2.39E-03 |
| U-238 [Surrogate 4] | 4.4700E+09 | 1.95E-09 | 2.23E-04 | 4.35E-03 |
| Co-60 [Surrogate 5] | 5.2710E+00 | 1.93E-07 | 0.00E+00 | 0.00E+00 |
| Cs-137 [Surrogate 8] | 3.0170E+01 | 2.44E-05 | 0.00E+00 | 0.00E+00 |

# 3.  TIER 1 CONTAMINANT SCREENING

Contaminants were screened using the attenuation factors developed in the transport simulations to identify those contaminants expected to contribute risk within definable time periods.  The Tier 1 screening is risk-based and involved first determining RBCs for design inventory contaminants in the design inventory. The RBCs are based on $10^{-4}$ risk for carcinogens and hazard index (HI) of 1 for non-carcinogens in groundwater at the downgradient compliance point. The MCL was also evaluated for those constituents for which MCLs have been promulgated. The contaminants presenting the largest apparent risk at the facility design inventory, and other contaminants identified as arriving in groundwater in the same time period, will be further assessed during the Tier 2 fate and transport effort. The results of screening for radiological and non-radiological contaminants in the design inventory are presented in the following subsections. The screening logic for Tier 1 and Tier 2 fate and transport evaluation and identification of preliminary groundwater RAO-based soil concentration limits is presented in Appendix C.  The exposure scenario used to develop the RBCs is presented in Appendix D, along with the summary of carcinogenic slope factors, reference doses for non-carcinogens, and MCLs for the contaminants identified for risk-based screening.

A summary of the contaminant screening activity is discussed in the following subsections. The contaminant screening is presented in greater detail in Appendices B and C. The screening resulted in identification of numerous constituents for which no groundwater RAO-based soil concentration limit was applicable. This is due to one, or both, of two important transport factors—the environmental half-life of individual constituents, and the relative mobility of constituents as defined by their partition coefficient.

## 3.1  Radionuclide Screening

All of the radioactive waste constituents were evaluated as carcinogens using carcinogenic slope factors published by the Environmental Protection Agency (EPA). The resultant modeled concentrations for the radioisotopes in the design inventory, along with the calculated risk are presented in Appendix B. Based on the screening, the isotopes identified in Table 3-1 were identified as the major risk contributors within temporally similar contaminant groups at the maximum design recharge rate of 0.0001 m/yr (i.e., presented $10^{-5}$ or greater risk within a discrete time period). These isotopes will be subjected to additional evaluation under Tier 2. The preliminary groundwater RAO-based concentrations (i.e., the lesser of calculated MCL, hazard index, or carcinogenic RBCs) for each radionuclide are presented in Appendix B. Appendix B presents the information used to apply the dilution/attenuation factors to the individual radionuclides and to subsequently account for radioactive decay to arrive at a representative expected peak concentration in groundwater for each constituent.

**Table 3-1.** Tier 1 screen major risk contributing radionuclides ($>10^{-5}$ risk).

| Recharge Rate | Elapsed Time (years) | Isotope | Calculated Risk for Isotope at Design Inventory (Decayed to Elapsed Time) | Selected Tier I RAO-Based Waste Soil Concentration (mg/kg) |
|---|---|---|---|---|
| 0.0001 m/yr | 2,000 - 500,000 | I129 | 5.99E-05 | 2.17E+03 |
| | >500,000 | U234 | 2.98E-05 | 6.56E+03 |
| | | U238 | 1.00E-05 | 6.02E+04 |
| | | Np237 | 1.07E-05 | 5.99E+03 |

## 3.2    Organic Compounds and Non-Radioactive Inorganics

Organic compounds and non-radioactive inorganic constituents of the design inventory were evaluated for their potential carcinogenic risk and their non-carcinogenic toxicity in addition to evaluation of applicable MCLs. The Tier 1 screening identified the constituents included in Table 3-2 that exhibited either estimated HI of 0.1 or greater, or carcinogenic risk of $10^{-5}$ or greater at the selected recharge rates.

The calculations performed to evaluate the migration and attenuation of the organic constituents were based on literature values for most input parameters. For some constituents (for example, nitroaniline and methyl naphthalene) no literature values for environmental half life and/or Koc were found. In this case, the migration and resultant groundwater concentrations for these constituents may be substantially overestimated if they are indeed subject to either partitioning onto the soil matrix or subject to predictable rates of decay. Similarly, some of the common inorganic ions and metallic elements (e.g., aluminum) that were identified as exhibiting elevated hazard indices, may not be readily soluble in the specific geochemistry of the landfill leachate. This will be further assessed in the Tier 2 evaluation.

The summary of the analysis of organic and inorganic constituents, in concert with the radionuclides previously discussed, is presented in Appendix B. Organic contaminants were decayed in the same manner as the radioisotopes, using literature values for environmental half-lives for individual constituents. Where closely related surrogate compounds could be identified, the surrogate half-lives were used for selected compounds in the design inventory. Literature values for several constituents could not be located. These constituents may require limitation through administrative control, or additional research to identify applicable characteristics.

**Table 3-2.** Summary of Tier 1 screening of non-radioactive constituents at maximum design recharge rate of 0.0001 m/yr. (Note: shaded boxes indicate exceedence of screening criteria HI = 1 or risk $>10^{-5}$.)

| Chemical Name | Risk Group Time period (yr) | Cumulative Cancer Risk at Design Inventory for all Non-Rad Constituents in Risk Group for Period | Cumulative HI at Design Inventory for all Non-Rad Constituents in Risk Group for Period | Non-carcinogenic HI at DI | Carcinogenic Risk at DI | Selected Tier I RAO-based Waste Soil Concentration (mg/kg) |
|---|---|---|---|---|---|---|
| Fluoride | 2000 - 500000 | 1.84E-07 | 2.53E+02 | 1.32E-01 | 0.00E+00 | 2.94E+01 |
| RDX | | | | 4.11E+00 | NA | 2.43E-01 |
| Cyanide | | | | 4.05E+00 | 0.00E+00 | 8.32E-02 |
| 2-Nitroaniline | | | | 5.84E+00 | 0.00E+00 | 4.66E-03 |
| 3-Nitroaniline | | | | 5.84E+00 | 0.00E+00 | 4.66E-03 |
| 4-Nitroaniline | | | | 5.84E+00 | 0.00E+00 | 4.66E-03 |
| Molybdenum | > 500000 | 1.08E-11 | 6.32E+00 | 1.05E-01 | 0.00E+00 | 9.70E+01 |
| Barium | | | | 6.17E+00 | 0.00E+00 | 2.91E+01 |
| 3-Methyl Butanal | | | | 0.00E+00 | 0.00E+00 | No Data |
| Decane, 3,4-Dimethyl | | | | 0.00E+00 | 0.00E+00 | No Data |
| Dimethyl Disulfide | | | | 0.00E+00 | 0.00E+00 | No Data |
| Eicosane | | | | 0.00E+00 | 0.00E+00 | No Data |
| Ethyl cyanide | | | | 0.00E+00 | 0.00E+00 | No Data |
| Heptadecane, 2,6,10,15-Tetra | | | | 0.00E+00 | 0.00E+00 | No Data |
| Octane,2,3,7-Trimethyl | | | | 0.00E+00 | 0.00E+00 | No Data |
| o-Toluenesulfonamide | | | | 0.00E+00 | 0.00E+00 | No Data |
| p-Toluenesulfonamide | | | | 0.00E+00 | 0.00E+00 | No Data |
| Tributylphosphate | | | | 0.00E+00 | 0.00E+00 | No Data |
| Undecane,4,6-Dimethyl- | | | | 0.00E+00 | 0.00E+00 | No Data |

# 4. RECOMMENDATIONS FOR TIER 2 FATE AND TRANSPORT ANALYSIS

Based on the results of the Tier 1 contaminant screening activity, the planned final cover for the ICDF should provide sufficient reduction in recharge through the landfill to prevent exceedence of the groundwater RAOs at the down-gradient compliance point. For those design basis minor constituents that indicate a potential for exceedence of the RAOs, administrative control through establishment of waste acceptance criteria (WAC) will provide sufficient protection of the environment. The following activities will be conducted as part of the Tier 2 modeling effort to support development of WAC:

- Additional research to identify transport parameters (e.g., Koc and/or environmental half-lives) for organic compounds that exceed Tier 1 criteria.

- Additional research to evaluate the expected range of background concentrations for metals and ions that exceed Tier 1 criteria. Metals and ions will be excluded from the Tier 2 analysis if the design inventory concentrations are within the range of background concentration based on existing data.

- The "Leachate Time Reduction Study," (DOE 2001c) will be integrated into the fate and transport simulation to provide parameters for geochemical controls on solubility. This may further reduce the number of constituents of potential concern.

- The preliminary "Leachate Time Reduction Study," (DOE 2001c) indicated that a potentially substantial mass of landfill contaminants may be subject to removal from the landfill system by planned leachate management activities during the operations and post-closure period. The Tier 2 activities will incorporate simulation of the removal of leachate from the landfill and evaluate the effects of that removal on the estimated groundwater concentrations. It is the intent of the design to place sludge residues from the evaporation ponds into the ICDF landfill before closure. Sediments will be dewatered and tested for meeting landfill disposal criteria.

The results of the Tier 2 fate and transport analysis will be presented in the 90% design waste acceptance criteria package.

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